Large-q expansion of the energy cumulants for the two-dimensional q-state Potts model

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Abstract

We have calculated the large-q expansion for the energy cumulants at the phase transition point in the two-dimensional q-state Potts model to the 23rd order in $1/\sqrt{q}$ using the finite lattice method. The obtained series allow us to give very precise estimates of the cumulants for $q > 4$ on the first order transition point. The result confirm us the correctness of the conjecture by Bhattacharya *et al.* on the asymptotic behavior of the cumulants for $q \to 4_+$.

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1 Introduction

It is a challenging problem to determine the order of the phase transition in the physical system where the order changes from the first order to the second one by a small variation of a parameter of the system. It is important to know how the quantities that remain finite at the first order transition point diverge or vanish when the parameter approaches the point at which the transition changes to the second order one. The q-state Potts model[1, 2] in two dimensions gives a good place to investigate the properties of the phase transition around such a point. It exhibits the first order phase transition for $q > 4$ and the second order one for $q \leq 4$. Many quantities of this model at the phase transition point $\beta = \beta_t$ are known exactly for $q > 4$, including the latent heat[3] and the correlation length[4, 5, 6], which vanishes and diverges, respectively, in the limit $q \to 4_+$. One the other hand physically important quantities such as the specific heat and the magnetic susceptibility at the transition point, which also increase to infinity as $q \to 4_+$, are not solved exactly. Bhattacharya *et al.*[7] made a stimulating conjecture on the asymptotic behavior of the energy cumulants including the specific heat at the first order transition point; the relation between the energy cumulants and the correlation in their asymptotic behavior at the first order transition point for $q \to 4_+$ will be the same as their relation in the second order phase transition for $q = 4$ and $\beta \to \beta_t$, which is well known from their critical exponents. If this conjecture is true not only in the q-state Potts model but also in other general physical systems with a phase transition whose order change from the first order to the second one when some parameter of the system is varied, it would give a good guide in investigating such systems.

Bhattacharya *et al.*[8] also made the large-q expansion of the energy cumulants to order 10 in $z \equiv 1/\sqrt{q}$ and they analyzed the series according to the conjecture, giving the estimates of the cumulants at the first order transition point for $q \geq 7$. The obtained estimates are at least one order of magnitude better than those given by other methods such as the Monte Carlo simulations[9] and the low-(and high-)temperature expansions[10, 11, 12], in spite of the fact that the maximum size of the diagrams taken into account in their large-q expansion is less than the correlation length for $q \lesssim 15$ while the Monte Carlo simulations are done carefully on the lattice with its size about 30 times as large as the correlation length and also the fact that the maximum size of the diagrams in their large-q expansion is as small as the half of the maximum size of the diagrams in the low-(and high-)temperature expansions These strongly suggest the correctness of the conjecture. The large-q series obtained by them are, however, not long enough to investigate the behavior of the energy cumulants for q closer to 4.

In this paper we will enlarge the large-q series for the energy cumulants at the transition point to order of 21 or 23 in z using the finite lattice method[13, 14, 15], instead of the standard diagrammatic method used by Bhattacharya *et al.*.

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The finite lattice method can in general give longer series than those generated by the diagrammatic method especially in lower spatial dimensions. In the diagrammatic method, one has to list up all the relevant diagrams and count the number they appear. In the finite lattice method we can skip this job and reduce the main work to the calculation of the expansion of the partition function for a series of finite size lattices, which can be done using the straightforward site-by-site integration[16, 17] without the diagrammatic technique. This method has been used mainly to generate the low- and high-temperature series in statistical systems and the strong coupling series in lattice gauge theory. One of the purposes of this paper is to demonstrate that this method is also applicable to the series expansion with respect to the parameter other than the temperature or the coupling constant. The long large-q series obtained here by the finite lattice method enables us to examine the conjecture by Bhattacharya *et al.* on the asymptotic behavior of the energy cumulants for q very close to 4. We can also give the estimates of the energy cumulants for each $q = 5, 6, 7, \cdots$ that are orders of magnitude more precise than the estimates by the previous works and they would serve as a target in investigating this model in various contexts, for example in testing the efficiency of a new algorithm of the numerical simulation. A brief note on this subject was already presented in [18], where we concentrated only on the specific heat.

The remainder of this paper is organized as follows. The algorithm of the finite lattice method to generate the large-q expansion of the free energy are given for the disordered phase in section 2 and for the ordered phase in section 3. The relation between the two algorithm is also discussed in section 3. The obtained series for the energy cumulants at the phase transition points are presented in section 4. In section 5 the series are analyzed to investigate the asymptotic behavior of the cumulants at $q \to 4_+$ as well as to make the estimation of the cumulants at various values of $q > 4$. In section 6 we conclude with a brief summary and a few remarks.

2 Algorithm in the disordered phase

The model is defined by the partition function

$$Z = \sum_{\{s_i\}} \exp\left(-\beta H\right), \qquad H = -\sum_{\langle i,j \rangle} \delta_{s_i, s_j} , \qquad (1)$$

where $\langle i, j \rangle$ represents the pair of nearest neighbor sites and s_i takes the values $1, 2, \cdots, q$. The phase transition point β_t is given by $\exp\left(\beta_t\right) - 1 = \sqrt{q}$. We first consider the free energy density in the disordered phase, which is given by

$$F_d(\beta) = \lim_{L_x, L_y \to \infty} (L_x L_y)^{-1} \ln Z_d(L_x, L_y) . \qquad (2)$$

Here the partition function $Z_d(L_x, L_y)$ in the disordered phase should be calculated for the $L_x \times L_y$ lattice with the free boundary condition as depicted in

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Fig.1. The large-q expansion of the partition function in this phase can be given through the Fortuin-Kasteleyn representation[19] as

$$Z_d(L_x, L_y) = q^{L_x L_y} \left[1 + \sum_{X \subseteq \Lambda_d} \phi(X) \right] , \qquad (3)$$

with

$$
\begin{aligned}
\phi(X) &= \left(e^\beta - 1 \right)^{b(X)} q^{c(X) - L_x L_y} \\
&= Y^{b(X)} z^{2[L_x L_y - c(X)] - b(X)} ,
\end{aligned}
\qquad (4)
$$

Here Λ_d is the set consisting of all bonds in the lattice, X is any subset of Λ_d and represents a configuration of bonds, excluding the empty set (the null configuration) which gives the leading contribution and is separated in the first term of Eq.(3). In Eq.(4) $Y \equiv (e^\beta - 1)/\sqrt{q}$, $z \equiv 1/\sqrt{q}$, $b(X)$ is the number of bonds in X and $c(X)$ is the number of clusters of sites in X. Two sites connected to each other by a bond belong to the same cluster (An isolated single site is a cluster). The $\phi(X)$ is called the *activity* of X. It is useful to note that the activity can be rewritten as

$$
\begin{aligned}
\phi(X) &= \left(e^\beta - 1 \right)^{b(X)} q^{-b(X) + l(X)} \\
&= Y^{b(X)} z^{b(X) - 2l(X)} ,
\end{aligned}
\qquad (5)
$$

where $l(X)$ is the number of independent closed loops formed by the bonds in X.

We define $H_d(l_x, l_y)$ for each $l_x \times l_y$ lattice ($1 \le l_x \le L_x, 1 \le l_y \le L_y$) as

$$H_d(l_x, l_y) = \ln \left[Z_d(l_x, l_y)/q^{l_x l_y} \right] , \qquad (6)$$

where $Z_d(l_x, l_y)$ is the partition function for the $l_x \times l_y$ lattice, again with the free boundary condition as shown in Fig.1. We next define $W_d(l_x, l_y)$ recursively as

$$
\begin{aligned}
W_d(l_x, l_y) = {} & H_d(l_x, l_y) \\
& - \sum_{\substack{l_x' \le l_x, l_y' \le l_y \\ (l_x', l_y') \ne (l_x, l_y)}} (l_x - l_x' + 1)(l_y - l_y' + 1) W_d(l_x', l_y') .
\end{aligned}
\qquad (7)
$$

Here the term with $l_x' = l_x$ and $l_y' = l_y$ should be excluded in the summation. Then the free energy density defined by Eq.(2) is given by[15]

$$F_d(\beta) = \ln(q) + \sum_{l_x, l_y} W_d(l_x, l_y) . \qquad (8)$$

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Now we have to know from what order in z the $W_d(l_x, l_y)$ starts. Only for this purpose, let us suppose to apply the standard cluster expansion[20, 21] based on the diagrams the large-q expansion for the free energy in the disordered phase. It should be stressed that in the practical calculation of the finite lattice method we need not perform this cluster expansion at all. A *polymer* is defined as a set X of bonds which satisfies the condition that there is no division of X into two sets X_1 and X_2 so that $\phi(X) = \phi(X_1)\phi(X_2)$. A set X composed of a single bond is a polymer. Below in this paragraph we discuss on the polymers that consists of two or more bonds. Now we define a *cluster of bonds* in X so that two bonds that are connected by a site belong to the same cluster. A polymer consisting of two or more bonds is composed of a single cluster of bonds, since a set of bonds composed of more than one disconnected clusters of bonds apparently does not satisfy the condition of a polymer. A cluster of bonds is a polymer if and only if the cluster of the bonds cannot be divided into tow or more clusters of bonds by cutting at any site that is shared by the bonds belonging to the cluster. We call such a cluster of bonds as *one-site irreducible*. In fact for a set X_r consisting of a *one-site reducible* cluster of bonds that can be divided into clusters $X_1, X_2, \cdots, X_n$ of bonds by cutting at a site, we have $\phi(X_r) = \phi(X_1)\phi(X_2)\cdots\phi(X_n)$, which implies that this set of bonds is not a polymer. For a cluster of bonds to be one-site irreducible, it is necessary that the bonds should form one or more closed loops and that each bond should belong to at least one of the loops, which we call *closed*. An example of a closed cluster of bonds is shown in Fig.2(a). For each closed cluster of bonds, the loop of the bonds which forms the perimeter of the whole cluster is called the *exterior boundary*. The exterior boundary for the closed cluster of bonds in Fig.2(a) is indicated in Fig.2(b). An *interior boundary* is a loop inside which all bonds are removed and we call the part of the cluster surrounded by the interior boundary as a *hole*. The closed cluster of bonds in Fig.2(a) has a hole with the interior boundary, as indicated in Fig.2(c). For a cluster of bonds to be one-site irreducible, not only should it be closed but also its exterior boundary has no crossing. If the exterior boundary has a crossing, as in Fig.3, the cluster of bonds is one-site reducible and is not a polymer. Thus a polymer is the closed cluster of bonds with its exterior boundary having no crossing. We list as an illustration in Fig.4 all the polymers that can be embedded within 3×3 lattice with their activities. The polymers are skipped that can be obtained by rotating and/or reflecting those in Fig.4. For later convenience we add some definitions concerning a polymer. A *concave corner* in the boundary of a polymer is the part of the boundary composed of two neighboring bonds that are bent perpendicular to each other toward the interior of the polymer. If two neighboring corners on the boundary are both concave, we call the two corners together with the bonds in a straight line connecting the two corners as a *concave part* of the boundary. Examples of the concave parts are given in Fig.5.

According to the theorem of the standard cluster expansion[20, 21], the free

energy for the $l_x \times l_y$ lattice is given by

$$\ln Z_d(l_x, l_y) = l_x l_y \ln q$$
$$+ \sum_{\{X_1, X_2, \cdots, X_n : connected\}} c(X_1, X_2, \cdots, X_n) \phi(X_1) \phi(X_2) \cdots \phi(X_n), \quad (9)$$

where the summation should be taken for every cluster of *connected* polymers $\{X_1, X_2, \cdots, X_n\}$ defined by the condition that there is no division of the cluster of polymers $\{X_1, X_2, \cdots, X_n\}$ into two clusters of polymers $\{X_1', X_2', \cdots, X_m'\}$ and $\{X_1'', X_2'', \cdots, X_{n-m}''\}$ $(m < n)$ so that $\phi(X_1 \cup X_2 \cup \cdots \cup X_n) = \phi(X_1' \cup X_2' \cup \cdots \cup X_m') \phi(X_1'' \cup X_2'' \cup \cdots \cup X_{n-m}'')$. (The 'cluster' of polymers here should be distinguished from the 'cluster' of sites in the Fortuin-Kasteleyn representation or the 'cluster' of bonds defined in the explanation of the polymers above.) The $c(X_1, X_2, \cdots, X_n)$ in Eq.(9) is the numerical factor that depends on the way how the clusters of polymers are connected, the details of which are not necessary here.

When a cluster of connected polymers can be embedded into the $l_x \times l_y$ lattice but cannot be embedded into any of its rectangular sub-lattices, we call it shortly to *fit into* the $l_x \times l_y$ lattice. Then we can prove the theorem[15] that the Taylor expansion of the $W_d(l_x, l_y)$ with respect to z includes the contribution from all the clusters of polymers in the standard cluster expansion that fit into the $l_x \times l_y$ lattice.

Now, according to this theorem, we can know the order of $W_d(l_x, l_y)$ in z by examining the clusters of connected polymers that fit into the $l_x \times l_y$ lattice. We first note that $W_d(1,1) = 0$ since the 1×1 lattice consists of a single site with no bond, so that no polymer can be embedded into this lattice, and $W_d(2,1) = W_d(1,2) = O(z)$ since the 2×1 or 1×2 lattice consists of two sites connected by one bond, so that a polymer composed of a single bond can be embedded into this lattice. We also note that $W_d(l_x, 1) = W_d(1, l_y) = 0$ for $l_x \geq 3$ or $l_y \geq 3$, because the corresponding lattice consists of the sites connected by bonds all on a straight line and the only clusters of polymers that fit into the lattice are those with each polymer composed only of a single bond and these polymers are not connected according to the definition of the connected polymers.

We next consider the order of $W_d(l_x, l_y)$ for $l_x \geq 2$ and $l_y \geq 2$. We first consider a cluster consisting of a single polymer that fits into the $l_x \times l_y$ lattice. If the polymer has a concave part in its exterior boundary we can add some bonds to make the part flat, obtaining a new polymer whose activity is changed by a factor of $Y^n z^{-1}$ with n the number of added bonds, so its order in z is lowered. This implies that a polymer that has concave part in the exterior boundary does not contribute to the lowest order term of $W_d(l_x, l_y)$ in z. Let us next consider the case when the polymer has some holes. The interior boundary surrounding each hole has at least one concave part. (We take the hole as the exterior of the polymer when we say 'concave' here.) We can add some bonds to make the

concave part flat, again obtaining a new polymer with the order of its activity in z lowered by a factor of z^{-1}. This implies that a polymer that has a hole does not contribute to the lowest order term of $W_d(l_x, l_y)$ in z. Thus the remaining polymers that have neither a concave part on the exterior boundary nor a hole in the interior give the contribution to the lowest order term of $W_d(l_x, l_y)$, examples of which are shown in Fig.6. They can be converted into each other by adding or removing pairs of bonds to their concave corners or from their convex corners, respectively. When each pair of bonds is added or removed the activity of the polymer is changed by Y^2 with its order in z unchanged. Hence we see that their orders are all the same; that is, the order of $z^{l_x+l_y-2}$. Next we consider a cluster of connected tow or more polymers that fits into the lattice. It is enough to take into account the clusters of polymers that do not have either a concave part on the boundary or a hole in the interior, since we are going to know the clusters of connected polymers that contributes to the lowest order term in z. Among the clusters of connected two or three polymers that fit into the lattice, those give the lowest order contribution in which the polymers touch each other only through their exterior boundary and each neighboring pair of polymers share only one bond, like Fig.7(a), and this type of clusters have the order of $z^{l_x+l_y+n-3}$ for the cluster of n polymers ($n = 2, 3$), which is higher than the lowest order contribution from the clusters composed of a single polymer. We note that a cluster of two or three polymers in which each neighboring pair of polymers share only one site, an example of which is given in Fig.7(b), is not connected according to the definition of the connected polymers. Among the cluster of connected more than four or more polymers that fit into the lattice, those give the lowest order contribution in which four of the polymers surround a plaquette and each neighboring pair of polymers share only one site, like Fig.8, and this type of clusters have the order of $z^{l_x+l_y+n-4}$ ($n \geq 4$) for the cluster of n polymers, which is also higher than the lowest order contribution from the clusters composed of a single polymer. In summary the lowest order term of $W_d(l_x, l_y)$ has the order of $z^{l_x+l_y-2}$ for $l_x \geq 2$ and $l_y \geq 2$, which comes from the clusters of a single polymer without a hole or a concave part fitting into $l_x \times l_y$ lattice. Thus in order to obtain the series to order z^N for the free energy density, we have only to take into account in Eq.(8) all the rectangular lattices that satisfy $l_x + l_y - 2 \leq N$.

We summarize the procedure of the finite lattice method to generate the large-q expansion series of the free energy density in the disordered phase.
1) Calculate the partition function $Z_d(l_x, L_y)$ defined by Eq.(3) as a power series of z to order z^N (and of Y in full order) for each $l_x \times l_y$ lattice with $l_x + l_y - 2 \leq N$. In these calculations use the transfer matrix method and integrate bond by bond[16, 17], which reduces the necessary CPU time and storage.
2) Calculate $H_d(l_x, l_y)$ defined by Eq.(6) as a power series of z by Taylor expanding $\ln Z_d(l_x, l_y)$ for each $l_x \times l_y$ lattice.
3) Calculate $W_d(l_x, l_y)$ defined recursively by Eq.(7) for each $l_x \times l_y$ lattice.
4) Sum up all the $W_d(l_x, l_y)$'s with $l_x + l_y - 2 \leq N$ according to Eq.(8) to obtain

the expansion series for the free energy density.

3   Algorithm in the ordered phase

Next we consider the large-q expansion of the free energy density $F_o(\beta)$ in the ordered phase, which is given by the same equation as Eq.(2) with the suffix d replaced by o where the partition function $Z_o(L_x, L_y)$ in the ordered phase should be calculated for the $L_x \times L_y$ lattice with the fixed boundary condition as depicted in Fig.9. The values of the spins on the boundary are all fixed to a single value among $1, 2, \cdots, q$.

By the duality the ordered and disordered free energy densities are related as

$$F_d(\beta) = F_o(\tilde{\beta}) + 2\ln((e^{\tilde{\beta}} - 1)/\sqrt{q})$$
$$\text{for} \qquad (e^\beta - 1)(e^{\tilde{\beta}} - 1) = q \ . \tag{10}$$

One method to obtain the large-q series for the energy cumulant $F_o^{(n)}$ at $\beta = \beta_t$ in the ordered phase is to use the relations

$$
\begin{aligned}
F_d^{(1)} + F_o^{(1)} &= 2(1 + z) \ , \\
F_d^{(2)} - F_o^{(2)} &= -z[F_d^{(1)} - F_o^{(1)}] \ , \\
F_d^{(3)} + F_o^{(3)} &= -3z[F_d^{(2)} + F_o^{(2)}] + (z - z^2)[F_d^{(1)} + F_o^{(1)}] \ , \\
F_d^{(4)} - F_o^{(4)} &= -6z[F_d^{(3)} - F_o^{(3)}] - (z - 6z^3)[F_d^{(1)} - F_o^{(1)}] \ , \\
F_d^{(5)} + F_o^{(5)} &= -10z[F_d^{(4)} + F_o^{(4)}] - (5z - 60z^3)[F_d^{(2)} + F_o^{(2)}] \\
&\quad + (z - z^2 - 24z^3 + 24z^4)[F_d^{(1)} + F_o^{(1)}] \ , \\
F_d^{(6)} - F_o^{(6)} &= -15z[F_d^{(5)} - F_o^{(5)}] - (15z - 300z^3)[F_d^{(3)} - F_o^{(3)}] \\
&\quad - (z - 90z^3 + 360z^5)[F_d^{(1)} - F_o^{(1)}] \ ,
\end{aligned}
\tag{11}
$$

which are derived directly from the duality relation (10). These were given in Ref.[8] except for the last one.

In spite of that, we give below the algorithm to generate the series for the free energy density in the ordered phase by the finite lattice method without relying on the duality relation. This algorithm will prove important when we are going to extend our work to generate the magnetization cumulants for instance, since they can be obtained by the derivative of the free energy density with respect to the external magnetic field and we have no longer duality relation for the free energy density in the presence of the external magnetic field. The large-q expansion of the partition function in this phase can be given also through the

Fortuin-Kasteleyn representation as

$$Z_o(L_x, L_y) = \left(e^\beta - 1\right)^{2L_x L_y - L_x - L_y} \left[1 + \sum_{\tilde{X}} \varphi(\tilde{X})\right] , \qquad (12)$$

with

$$\begin{aligned}
\varphi(\tilde{X}) &= \left(e^\beta - 1\right)^{-b(\tilde{X})} q^{c(\tilde{X})} \\
&= \tilde{Y}^{b(\tilde{X})} z^{b(\tilde{X}) - 2c(\tilde{X})} .
\end{aligned} \qquad (13)$$

Here $\tilde{X}$ is a configuration of the removed bonds and we also use $\tilde{X}$ to represent the set of removed bonds. In the leading configuration for the fixed boundary condition all the pairs of nearest neighbor sites are connected by the bonds and there is no removed bonds ($\tilde{X}$ is the empty set), and its contribution is separated as the first term of Eq.(12). In Eq.(13) $\tilde{Y} \equiv \sqrt{q}/(e^\beta - 1)$ and $b(\tilde{X})$ is the number of bonds in $\tilde{X}$ and $c(\tilde{X})$ is the number of clusters of sites in the configuration of bonds with $\tilde{X}$ removed without taking into account the clusters including the sites on the boundary. We define $H_o(l_x, l_y)$ for each $l_x \times l_y$ lattice $(1 \leq l_x \leq L_x, 1 \leq l_y \leq L_y)$ as

$$H_o(l_x, l_y) = \ln \left[Z_o(l_x, l_y) / \left(e^\beta - 1\right)^{2l_x l_y - l_x - l_y}\right] , \qquad (14)$$

where $Z_o(l_x, l_y)$ is the partition function for the $l_x \times l_y$ lattice, again with the fixed boundary condition as shown in Fig.9. We next define $W_o(l_x, l_y)$ recursively in the same way as in Eq.(7). Then the free energy density in the ordered phase is given by

$$F_o(\beta) = 2 \ln \left(e^\beta - 1\right) + \sum_{l_x, l_y} W_o(l_x, l_y) . \qquad (15)$$

It is useful to compare now the large-q expansions by the finite lattice method for the disordered phase presented in the previous section and for the ordered phase presented here. We first note that the lattice with the free boundary condition in Fig.1 and the lattice with the fixed boundary condition in Fig.9 are dual to each other in the sense that each site of one lattice is located at the center of a plaquette of the other lattice, when the two lattices have the same size. We denote $X \sim \tilde{X}$ as the relation between the configuration X of the bonds on the lattice with the free boundary condition and the configuration $\tilde{X}$ of the removed bonds on the lattice with the fixed boundary condition, if the location of each bond (identified with its center) in X coincides with the location of each corresponding removed bond (also identified with its center) in $\tilde{X}$ (see Fig.10(a) and (b)). Then, the number $l(X)$ of independent closed loops for each configuration X in Eq.(5) is equal to the number $c(\tilde{X})$ of clusters of sites in the

configuration with $\tilde{X}$ removed in (13) for $\tilde{X} \sim X$ (see Fig.10(a) and (b)), so that $\phi(X) = \varphi(\tilde{X})$ when $Y = \tilde{Y}$. We therefore know from Eq.(3), (6), (12) and (14) that $H_d(l_x, l_y; Y, z) = H_o(l_x, l_y; \tilde{Y}, z)$ when $Y = \tilde{Y}$, hence the same is true for $W_d(l_x, l_y; Y, z)$ and $W_o(l_x, l_y; \tilde{Y}, z)$. Thus $W_o(l_x, l_y)$ has the same order in z as $W_d(l_x, l_y)$, that is, the order of $z^{l_x + l_y - 2}$. So in order to generate the series to order z^N we have only to take into account the rectangular lattices with $l_x + l_y - 2 \le N$ in Eq.(15). This conclusion can also be reached by repeating the discussion based on the standard cluster expansion using the diagrams. The discussion goes completely in parallel with those given for the disordered phase in the previous section if the set of bonds X representing the configuration of bonds for the disordered phase is replaced by the set of removed bonds $\tilde{X}$ for the ordered phase.

The relation of $W_d(l_x, l_y; Y, z) = W_o(l_x, l_y; \tilde{Y}, z)$ for $Y = \tilde{Y}$ also implies that the free energy densities $F_d(\beta)$ given by Eq.(8) and $F_o(\tilde{\beta})$ given by Eq.(15) satisfy the duality relation (10), because the condition that $Y = \tilde{Y}$ is equivalent to the condition for β and $\tilde{\beta}$ in the duality relation in Eq.(10).

4   Series

The algorithms in the previous two sections give the large-q expansion of the free energy density at the arbitrary inverse temperature β. The energy cumulants can be obtained by taking its derivative with respect to β. If we are interested only in the energy cumulants at the phase transition point, as is the case here, we can set $Y = 1 + y$ and $\tilde{Y} = 1 + \tilde{y}$ (with $y = 0$ and $\tilde{y} = 0$ at $\beta = \beta_t$)[22], then in order to obtain the n-th cumulant we have only to keep the expansion with respect to y to order y^n as

$$F_d^{(n)} = \left. \frac{d^n}{d\beta^n} F_d(\beta) \right|_{\beta = \beta_t} = \sum_m a_m^{(n)} z^m , \qquad (16)$$

using $\frac{d}{d\beta} = (1 + y + z)\frac{d}{dy}$ and

$$F_o^{(n)} = \left. \frac{d^n}{d\beta^n} F_o(\beta) \right|_{\beta = \beta_t} = \sum_m b_m^{(n)} z^m , \qquad (17)$$

using $\frac{d}{d\beta} = [1 + \tilde{y} + (1 + \tilde{y})^2 z]\frac{d}{dy}$.

Using this procedure we have calculated the series to order $N = 23$ in z for the n-th order cumulants with $n = 0, 1, 2$ and to order $N = 21$ for the cumulants with $n = 3, \cdots, 6$. The coefficients of the series are listed in Table 1.1 and 1.2 for the disordered phase and in Table 2.1 and 2.2 for the ordered phase. We have applied the finite lattice method both in the ordered and disordered phases without relying on the duality relations (11) for the cumulants. We have checked that all of the $W_d(l_x, l_y)$ and $W_o(l_x, l_y)$ with $l_x + l_y - 2 \le N$ have the correct

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order in z as described in the previous two sections. The obtained series for the zeroth and first cumulants (i.e. the free energy and the internal energy) agree with the expansion of the exactly known expressions. The coefficients for $F_o^{(n)}$ agree with those by Bhattacharya *et al.* to order 10. We have also checked that the series satisfy the duality relations (11) for the cumulants.

5 Analysis

In this section we analyze the large-q series for the energy cumulants presented in the previous section. The asymptotic behavior of the energy cumulants at $\beta = \beta_t$ for $q \to 4_+$ was conjectured by Bhattacharya *et al.*[7] as follows. It is well known that there is an asymptotic relation between the energy cumulants and the correlation length ξ for $\beta \to \beta_t$ at $q = 4$ as

$$F_d^{(n)}, (-1)^n F_o^{(n)} \sim A \frac{\Gamma\left(n - \frac{4}{3}\right)}{\Gamma\left(\frac{2}{3}\right)} \xi^{3n/2-2}, \tag{18}$$

with the constant A that is independent of n. This relation comes from the fact that the critical exponents of the correlation length and the specific heat in the second order phase transition are $\nu = 2/3$ and $\alpha = 2/3$, respectively, for $q = 4$. Their conjecture claims that the relation (18) is also held as the asymptotic relation between the energy cumulants and the correlation length at the first order phase transition point for $q \to 4_+$. Then, from the known asymptotic behavior of the correlation length at the first order phase transition point for $q \to 4_+$ as[6]

$$\xi \sim \frac{1}{8\sqrt{2}} x \, ,$$

where $x \equiv \exp\left(\frac{\pi^2}{2\theta}\right)$ with θ defined by $2\cosh\theta \equiv \sqrt{q}$ ($\theta \sim \sqrt{q-4}/2$ for $q \to 4_+$), the conjecture implies that the asymptotic form of the energy cumulants in the limit of $q \to 4_+$ is given by

$$F_d^{(n)}, (-1)^n F_o^{(n)} \sim \alpha B^{n-2} \frac{\Gamma\left(n - \frac{4}{3}\right)}{\Gamma\left(\frac{2}{3}\right)} x^{3n/2-2} \, . \tag{19}$$

We notice that the constants α and B should be independent of n and from the duality relations (11) that they should be common to the ordered and disordered phases.

To analyze the large-q series for these quantities, Bhattacharya *et al.* used a sophisticated method. Let $f(z)$ be a function that has the asymptotic behavior of the right hand side of Eq.(19). Then $\theta \ln f(z)$ is a regular function of z except for the possible terms proportional to the inverse powers of x, which vanishes rapidly when θ approaches zero. Although θ itself cannot be expanded as the power series of z since θ diverge at $z = 0$, the quantity $1 - e^{-\theta} =$

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$1 - 2z/(\sqrt{1 - 4z^2} + 1)$ behaves like θ for $\theta \to 0$ and can be expanded as a power series of z. Then one may expect that $(1 - e^{-\theta}) \ln f(z)$ will be a smooth function of z and it's Padé approximant will give a convergent result for $q \to 4_+$. In fact using the 10th order series Bhattacharya *et al.* found that the Padé approximants of $F^{(2)}$ give convergent results for $q \gtrsim 7$. The obtained results were more precise than the results of the Monte Carlo simulations[9] and the low-(or high-)temperature series[10, 11, 12] as mentioned in the introduction and exhibits rather flat behavior of $F^{(2)}/x$ around $7 \lesssim q \lesssim 10$, suggesting the correctness of the asymptotic behavior (19) for $n = 2$ with $\alpha \sim 0.76$. If we use our longer 23rd order series of $F^{(2)}$ to repeat these Padé analysis, we find that the convergent region of q is extended down to $q \sim 5$, with the accuracy of a few percent at $q = 5$ and the data of $F^{(2)}/x$ is rather flat for $5 \lesssim q \lesssim 10$, which gives a stronger support to the conjecture that $F^{(2)}$ is approaching it's asymptotic form (19).

We, however, adopt here another method of the analysis that is simpler and more efficient. The latent heat $\mathcal{L}$ has the exact asymptotic form as[7]

$$\mathcal{L} \sim 3\pi x^{-1/2} ,$$

so, if $F^{(n)}$ has the asymptotic form of Eq.(19), the product $F^{(n)}\mathcal{L}^p$ is a smooth function of z for $q \to 4_+$ when $p = 3n - 4$, while it behaves like some positive or negative powers of x and has an essential singularity with respect to z at $q = 4$ when $p \neq 3n - 4$. Thus if we try the Padé approximation of $F^{(n)}\mathcal{L}^p$ it will lead to a convergent result for $p = 3n - 4$, while the approximants will scatter when p is off this value. In the Padé approximation of $F^{(n)}\mathcal{L}^p$ the series for the ordered and disordered phases should be treated in a slightly different way, corresponding to the difference of the lowest order of the series; the series for the ordered phase starts from the order of z^2, while the series for the disordered phase starts from the order of z. Thus we should solve the following equation:

$$F^{(n)}\mathcal{L}^{3n-4} = z^r P_M(z)/Q_L(z) + O(z^{M+L+r+1}) , \qquad (20)$$

where r is 2 for the ordered phase and 1 for the disordered phase, and $P_M(z)$ and $Q_L(z)$ are polynomials of order M and L respectively with $M + L + r = N$ where N is the truncated order of the series. Fig.11 is the result of this analysis of $F_d^{(2)}\mathcal{L}^p$ for $q = 4$. We see very clearly that the Padé approximants have the best convergence at $p = 2.00(1)$ and the convergence becomes bad rapidly when p leaves this value. All the other approximants for $F_{d,o}^{(n)}\mathcal{L}^p$ have similar behaviors with respect to p with the best convergence at $p = 3n - 4$, although we do not show them in figures. These results are enough to convince us that $F_{d,o}^{(n)}$ has the asymptotic behavior that is proportional to $x^{3n/2-2}$.

Then we calculate the amplitude of $F^{(n)}$ for each q by taking the Padé approximants of $F^{(n)}\mathcal{L}^{3n-4}$ and multiplying $\mathcal{L}^{4-3n}$ that is calculated from its exact expression. Usually a diagonal approximant (that is, $M = L$) or it's

neighborhood produces good estimates. We, however, adopt here all the approximants with $M \geq 8$ and $L \geq 8$, since we have found in this case that each of these approximants is scattered almost randomly around their average value and we have found no reason to give a special position only to the diagonal approximant. Some denominators of the approximants have zero at $z < 1/2$ ($q > 4$) and we have excluded such approximants. The results for $n = 2, \cdots, 6$ in the ordered and disordered phases are listed in Table 3–6 for integer values of $q \geq 5$, with the second energy cumulant transformed to the specific heat by multiplying β_t^2. In Figs. 12-16, we also plot $|F^{(n)}|/x^{\frac{3n}{2}-2}$ versus θ for $n = 2$–6, respectively. In these figures the dotted and dashed lines indicate the errors for the disordered and ordered phases, respectively. In these tables and figures the given errors represent the magnitude of the fluctuation in the data of the Padé approximants.

In any case, the estimates have surprisingly high accuracy. Our data are orders of magnitude more precise than the result of the Monte Carlo simulation by Janke and Kappler[9] for $q = 10, 15, 20$ (also listed in Table 3–6), which was performed carefully in large enough lattices checking the finite size effects, and they are consistent with each other except for small differences in the data of the 5th and 6th cumulants for the ordered phase. On the other hand, the results of the low-temperature series[12] (also listed in Table 3 and 4) are inconsistent with these. This would be because we do not have the correct knowledge (or conjecture) of the possible singularity structure of the cumulants at some $\beta \leq \beta_t$ in extrapolating the low-temperature series toward $\beta = \beta_t$. We should emphasize that the values of the specific heat has an accuracy of about 0.1 percent at $q = 5$ where the correlation length is as large as 2500 lattice spacing[6] and there is no previous data to be compared with, and of a few percent even at the limit of $q = 4$ where the correlation length diverges. The accuracy is better by a factor of more than 10 when compared with the result of using the Padé approximation for $(1 - e^{-\theta}) \ln F^{(n)}$. The reason for this is the following. Let us suppose that the Padé approximants gives estimates of $F^{(n)} \mathcal{L}^{3n-4} = c(1 \pm \delta)$ and $(1 - e^{-\theta}) \ln F^{(n)} = c'(1 \pm \delta')$, then the estimate of $F^{(n)}$ from the former would also have an ambiguity factor of $1 \pm \delta$, while the estimate of $F^{(n)}$ from the latter would have an ambiguity factor of $e^{\pm c'\delta'/\theta}$, which grows up for the plus sign and shrinks to zero for the minus sign when $\theta \to 0 (q \to 4_+)$.

Next we determine the constant α and β in the asymptotic form (19) for $q \to 4_+$. The constants α can be determined by the value of $F^{(2)}/x$ in the limit of $q \to 4_+$. We read from Fig.12 that

$$\alpha = 0.073 \pm 0.002 .$$

On the other hand, the constant B is given by the asymptotic value of the following combination for $n \geq 3$:

$$\left\{ \frac{\Gamma \left(n - \frac{4}{3} \right) |F^{(n)}|}{\Gamma \left(\frac{2}{3} \right) F^{(2)}} \right\}^{\frac{1}{n-2}} x^{-\frac{3}{2}} . \tag{21}$$

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Their asymptotic values should be common to each n. The behavior of the quantity in Eq.(21) for the ordered and disordered phases are given in Fig.17 and 18 respectively. The graphs for $n = 3$ and $n = 4$ show clear convergence even at $\theta = 0$ giving the value of B very close to each other, that is, $B \sim 0.38(3)$ We also notice that, although the results for $n = 5$ and $n = 6$ have considerably large errors in the small θ region so we cannot say anything definite, the values of the quantity in Eq.(21) at the points where the errors begin to grow are also close to this value of $0.38(3)$. Thus we may estimate the constant B as

$$B = 0.38 \pm 0.03 \ .$$

In conclusion the Padé data of the large-q series convince us that the conjecture (19) for the asymptotic form is true at least for $n = 2, 3$ and 4 and suggest its correctness for $n = 5$ and 6.

6   Summary

The finite lattice method were applied to generate the large-q expansion of the n-th energy cumulants ($n = 0, 1, \cdots, 6$) at the phase transition point for the ordered and disordered phases in the two-dimensional q-state Potts model. It enabled us to extend the series to the 23rd order in $z = 1/\sqrt{q}$ for $n = 0, 1, 2$ and to the 21st order for $n = 3, \cdots, 6$ from the 10th order generated by Bhattacharya *et al.* using the standard diagrammatic method. We made the Padé analysis of the series for the product of each cumulant and some powers of the latent heat that is expected to be a smooth function of z if the conjecture by Bhattacharya *et al.* is true that the relation between the cumulants and the correlation length in the asymptotic behavior for $\beta \to \beta_t$ at $q = 4$ will be kept in their asymptotic behavior at the first order transition point for $q \to 4_+$. It allowed us to present very precise estimates of the cumulants at the transition point for $q > 4$. The accuracy of the estimates is orders of magnitude higher than the results of the Monte Carlo simulations and the low-(and high-) temperature series for $q \gtrsim 7$, and for instance of about 0.1 percent at $q = 5$ where the correlation length is as large as a few thousand lattice spacing and there is no previous data to be compared with, and of a few percent even at the limit of $q = 4$ where the correlation length diverges. The resulting asymptotic behavior of the cumulants for q close to 4 is consistent with the conjecture not only for the second cumulant (or the specific heat) but also for the higher cumulants.

Now it is quite natural to ask whether the conjecture by Bhattacharya *et al.* for the energy cumulants can be extended to other quantities such as the magnetization cumulants at the first order phase transition point that diverge in the limit of $q \to 4_+$. We can expect that the long series of the large-q expansion for the quantities would serve to answer this question as the long series for the energy cumulants did in this paper. It is rather straightforward to extend the large-q expansion by the finite lattice method to such quantities.

They are obtained in general by the derivative of the free energy density in the presence of appropriate external fields or sources, which can also be given by the algorithm of the finite lattice method described in this paper with a minor modification. Since no duality relation is known for the free energy density in the presence of the external fields, both of the algorithms presented here for the ordered and disordered phases will be useful, especially in what type of the boundary condition one should adopt for the finite size lattices. The calculation and analysis of the large-q series for the magnetization cumulants are now in progress.[23]

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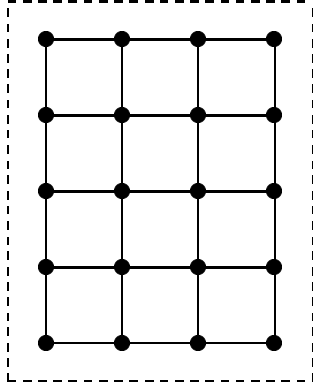
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Figure 1: $L_x \times L_y$ lattice (in this figure $L_x = 4$ and $L_y = 5$) with the free boundary condition for the disordered phase.
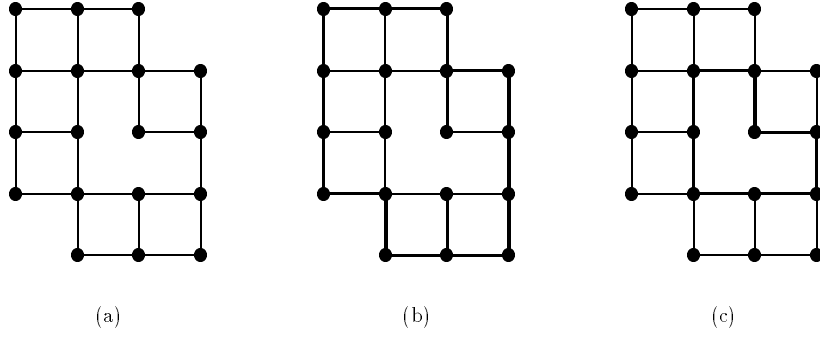
Figure 2: (a) Example of a closed cluster of bonds with a hole. (b) The same as (a) with the exterior boundary highlighted by thick lines. (c) The same as (a) with the interior boundary highlighted by thick lines.
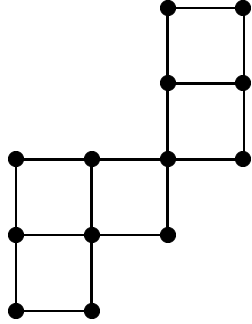

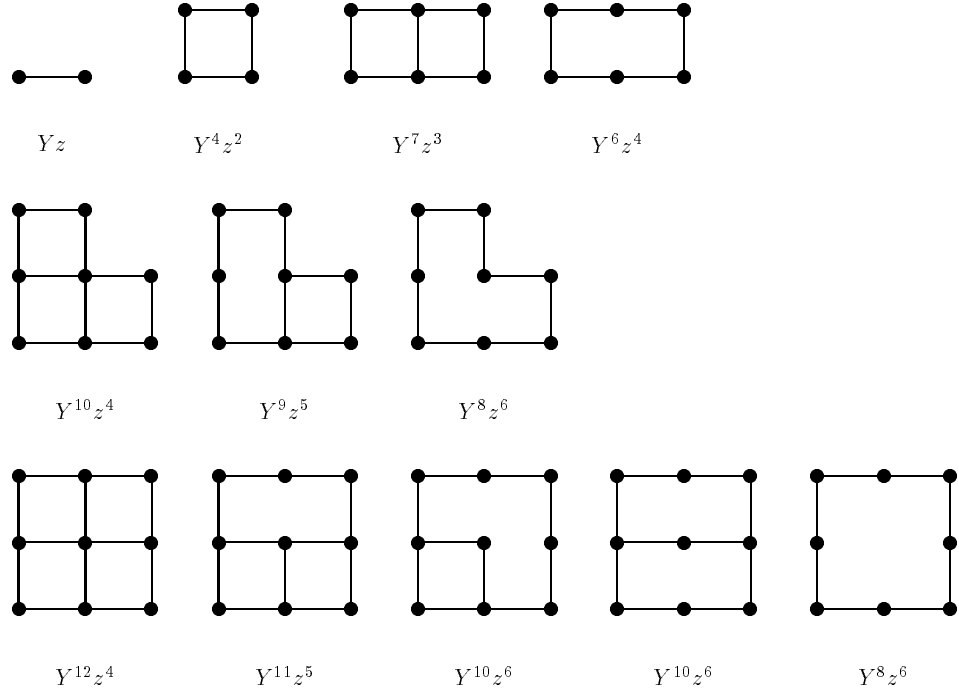Figure 3: Example of a polymer whose exterior boundary has a crossing.

Figure 4: All the polymers that can be embedded within 3×3 lattice with their activities.
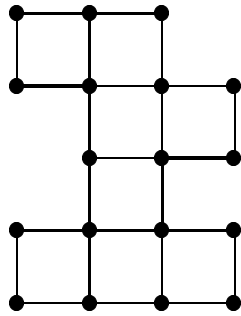

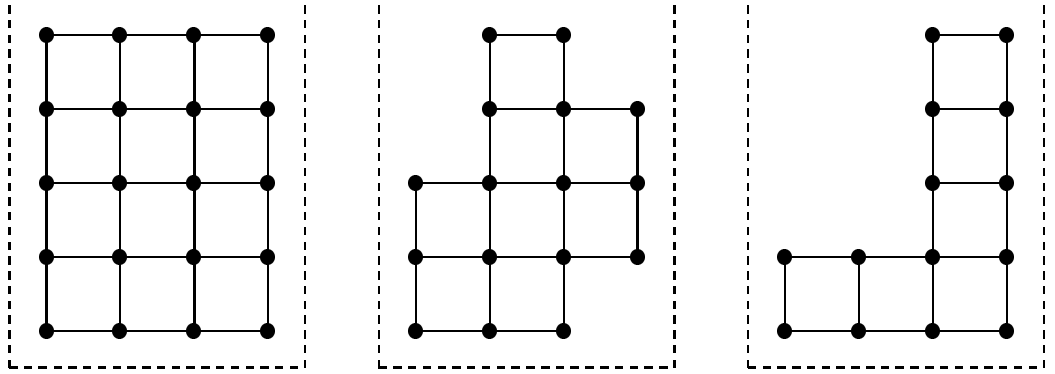Figure 5: Example of a polymer with two concave parts highlighted by thick lines.

Figure 6:   Examples of the cluster consisting of a single polymer that contribute to the lowest order term of the $W_d(l_x, l_y)$ with $l_x = 4$ and $l_y = 5$.

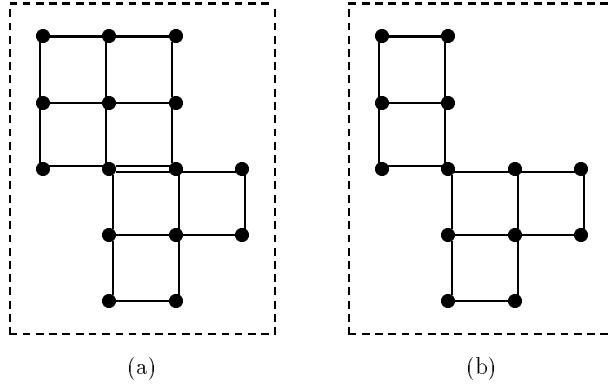(a)   (b)

Figure 7:   (a) Example of the cluster consisting of connected two polymers that share only one bond. (b) Example of the cluster consisting of disconnected two polymers that share only one site.
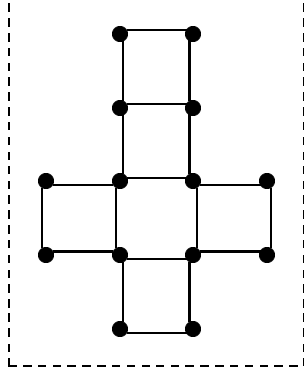
Figure 8: Example of the cluster consisting of connected four polymers that surround a plaquette and each neighboring pair of polymers share only one site.
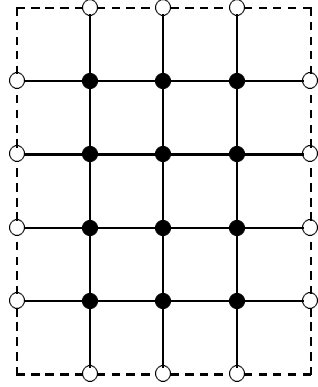

Figure 9: $L_x \times L_y$ lattice (in this figure $L_x = 4$ and $L_y = 5$) with the fixed boundary condition for the ordered phase. The spins of the sites on the boundary (open circles) are fixed to a single value among $1, 2, \cdots, q$.
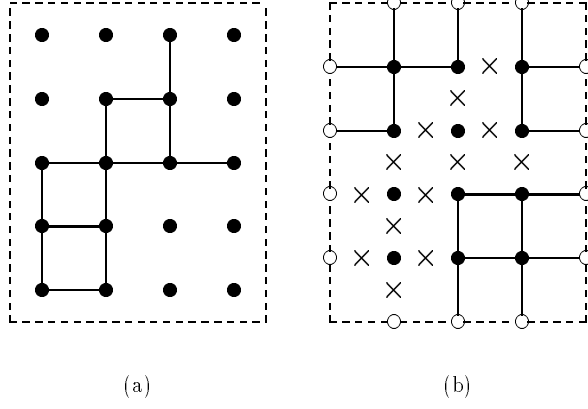
(a)   (b)

Figure 10:   (a) Example of the configuration X of bonds (solid lines) for the free boundary condition. (b) The configuration $\tilde{X}$ of removed bonds (crosses) for the fixed boundary condition with $X \sim \tilde{X}$.
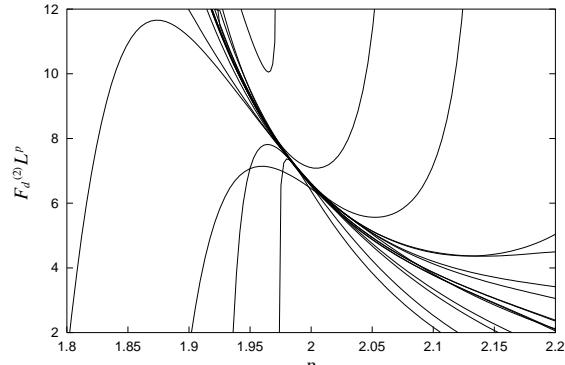
Figure 11:   Padé approximants of $F_d^{(2)}\mathcal{L}^p$ at $q = 4$ with $M \geq 9$ and $L \geq 9$ plotted versus p.
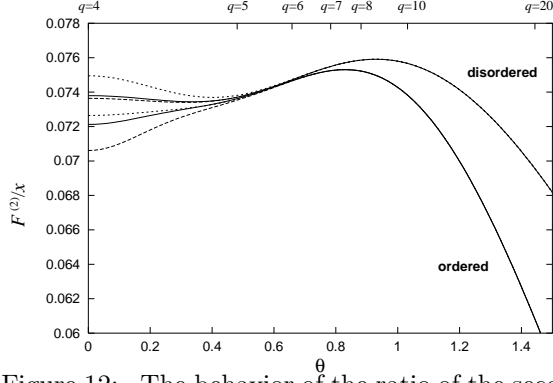
Figure 12:   The behavior of the ratio of the second energy cumulants $F_{d,o}^{(2)}$ to x.

Figure 13:   The behavior of the ratio of the absolute value of the third energy cumulants $|F_{d,o}^{(3)}|$ to $x^{5/2}$.
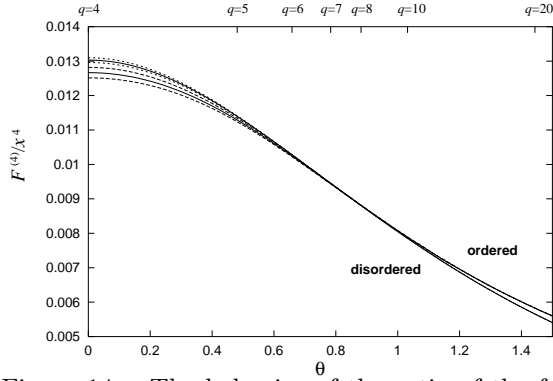
Figure 14:   The behavior of the ratio of the fourth energy cumulants $F_{d,o}^{(4)}$ to x^4.

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Figure 15: The behavior of the ratio of the absolute value of the fifth energy cumulants $|F_{d,o}^{(5)}|$ to $x^{11/2}$.
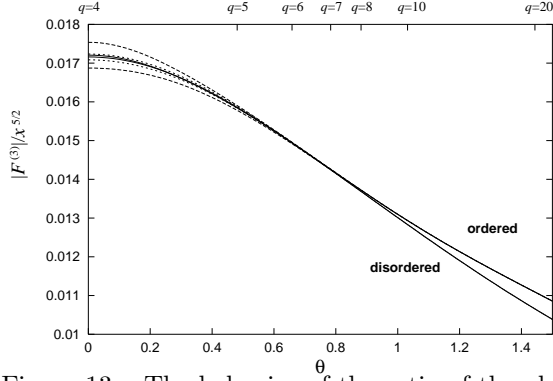

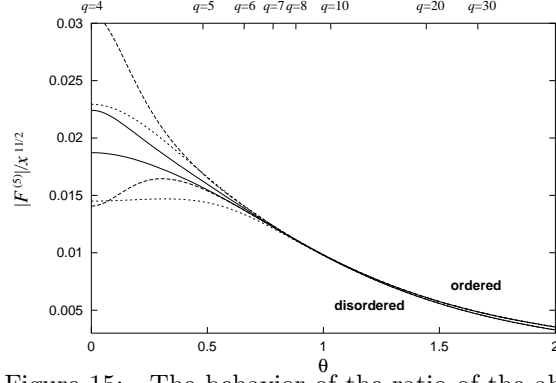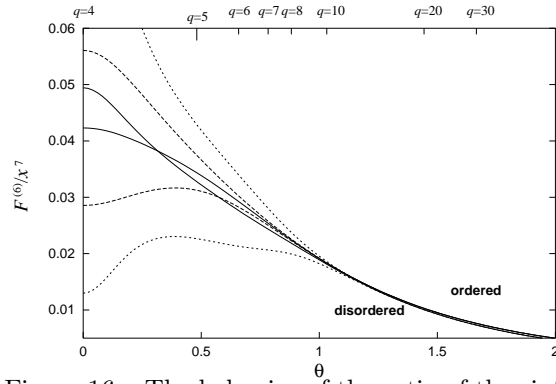Figure 16: The behavior of the ratio of the sixth energy cumulants $F_{d,o}^{(6)}$ to x^7.
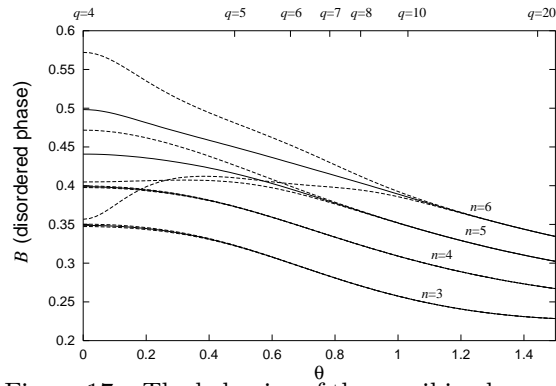
Figure 17: The behavior of the comibined quantity of Eq.(21) in the disordered phase.

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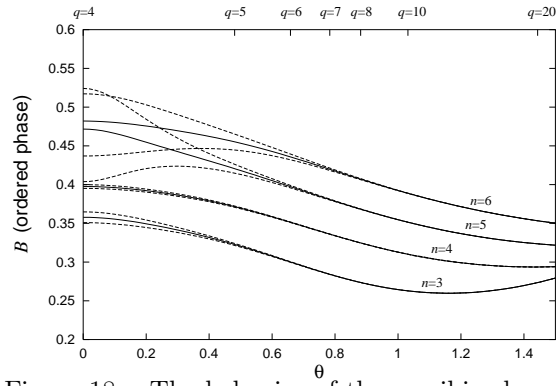
Figure 18:   The behavior of the comibined quantity of Eq.(21) in the ordered phase.

Table 1.1: The large-q expansion coefficients $a_m^{(n)}$ for the n-th energy cumulants of the free energy at $\beta = \beta_t$ in the disordered phase ($n = 1$–4).

m	$a_m^{(1)}$	$a_m^{(2)}$	$a_m^{(3)}$	$a_m^{(4)}$
0				
1	2	2	2	2
2	4	14	58	242
3	−2	26	338	3026
4	2	118	2474	37186
5	−6	250	11490	291946
6	4	894	55506	2068914
7	−16	1936	219404	12144136
8	6	6160	876384	65992348
9	−38	13538	3127818	322997186
10		39774	11161914	1494569130
11	−76	88360	37125056	6470376688
12	−56	245188	122847224	26851465312
13	−96	547468	387657840	106378391164
14	−348	1457976	1214792028	407805474096
15	156	3264012	3679570740	1510368315660
16	−1634	8410284	11061186460	5448643138308
17	1946	18868858	32420680250	19136730128506
18	−6852	47391870	94306690802	65779858359354
19	10744	106180532	269004235012	221297704673276
20	−27004	261607968	761823806996	731233034945892
21	48492	586199668	2124082332388	2373735516063508
22	−102226	1415498882		
23	199386	3174300542		

Table 1.2:   The large-q expansion coefficients $a_m^{(n)}$ for the n-th energy cumulants of the free energy at $\beta = \beta_t$ in the disordered phase ($n = 5, 6$).

m	$a_m^{(5)}$	$a_m^{(6)}$
0		
1	2	2
2	994	4034
3	24338	186626
4	488162	5995138
5	5985042	110362330
6	60977034	1583071794
7	503300684	17852715736
8	3668770296	171621163420
9	23690762442	1432076136578
10	140396232786	10720828033434
11	768231161504	72985931413600
12	3949989951344	459566465021728
13	19184686377744	2701568006995708
14	88891085678652	14974796851686096
15	394525773133188	78777820375010652
16	1687573606453276	395842580467193364
17	6978567585546266	1908650742049266298
18	28012258546890218	8869906520648194890
19	109405587397512484	39863282911219604012
20	416940286121010524	173802434948834045508
21	1553287387425965092	737013278292605504308

Table 2.1: The large-q expansion coefficients $b_m^{(n)}$ for the n-th energy cumulants of the free energy at $\beta = \beta_t$ in the ordered phase ($n = 1$–4).

m	$b_m^{(1)}$	$b_m^{(2)}$	$b_m^{(3)}$	$b_m^{(4)}$
0	2			
1				
2	−4	16	−64	256
3	2	34	−430	3778
4	−2	114	−2654	41778
5	6	254	−12186	322670
6	−4	882	−57018	2210982
7	16	1944	−224732	12819264
8	−6	6128	−888024	68657204
9	38	13550	−3164682	333583598
10		39698	−11243178	1532324246
11	76	88360	−37363472	6604807168
12	56	245036	−123377384	27298396784
13	96	547356	−389128512	107855738700
14	348	1457784	−1218076500	412466192928
15	−156	3263316	−3688318020	1524965526804
16	1634	8410596	−11080768444	5492850472332
17	−1946	18865590	−32471142890	19269581858838
18	6852	47395762	−94419894146	66169209300214
19	−10744	106166828	−269288597908	222430064188868
20	27004	261629456	−762460849076	734462791941548
21	−48492	586145660	−2125652044660	2382881224028156
22	102228	1415594740		
23	−199212	3174081000		

Table 2.2: The large-q expansion coefficients $b_m^{(n)}$ for the n-th energy cumulants of the free energy at $\beta = \beta_t$ in the ordered phase ($n = 5, 6$).

m	$b_m^{(5)}$	$b_m^{(6)}$
0		
1		
2	-1024	4096
3	-29518	218914
4	-556382	6813714
5	-6773994	126069374
6	-67122114	1774583142
7	-546094604	19774354944
8	-3918393456	187361651588
9	-25037212842	1545876302510
10	-146961943266	11451708807878
11	-798499755344	77296110810160
12	-4080741048224	483066658347536
13	-19726182681504	2822025943834956
14	-91033421848212	15558449192797824
15	-402728474968788	81476650613568516
16	-1717926911825116	407801271671111676
17	-7087982430811466	1959732852092226390
18	-28396321463796218	9080903533904186662
19	-110725077538793524	40709407799692233428
20	-421377562607301884	177104383529723970956
21	-1567944342623768692	749588012269824549980

Table 3: Estimates of the specific heat C_d for the disordered phase in comparison with the low-temperature series and the Monte Carlo simulations.

q	large-q	low-temp.	Monte Carlo
5	2889.1(41)		
6	205.930(55)		
7	68.7370(52)	68.01(47)	
8	36.9335(11)	30.17(6)	
9	24.58756(35)	20.87(5)	
10	18.38542(17)	16.294(34)	18.437(40)
15	8.6540342(98)	8.388(4)	8.6507(57)
20	6.132159678(47)	6.0645(69)	6.1326(4)
30	4.29899341467(73)	4.2919(51)	

Table 4: Estimates of the specific heat C_o for the ordered phase in comparison with the low-temperature series and the Monte Carlo simulations.

q	large-q	low-temp.	Monte Carlo
5	2885.8(34)		
6	205.780(32)		
7	68.5128(22)	52.98(61)	
8	36.62347(31)	28.47(47)	
9	24.203436(65)	20.03(27)	
10	17.937801(18)	15.579(83)	17.989(40)
15	7.99645871(22)	7.721(28)	7.999(3)
20	5.360768767(13)	5.2913(53)	5.3612(4)
30	3.41289525542(28)	3.4012(10)	

Table 5: Estimates of the energy cumulants $F_d^{(n)}$ for the disordered phase ($n = 3$–6). The values in the brackets are the data of the Monte Carlo simulations.

q	$F_d^{(3)}$	$F_d^{(4)}$
5	$2.1597(27) \times 10^9$	$7.4380(99) \times 10^{15}$
6	$2.04752(87) \times 10^6$	$1.07367(47) \times 10^{11}$
7	$9.8404(16) \times 10^4$	$8.2877(14) \times 10^8$
8	$16420.4(11)$	$4.69139(37) \times 10^7$
9	$4880.80(16)$	$6.69421(26) \times 10^6$
10	$2002.017(32)$	$1.600281(33) \times 10^6$
	$[2015(26)]$	$[1.583(64) \times 10^6]$
15	$176.78507(17)$	$32323.501(59)$
	$[176.01(76)]$	$[2.93(20) \times 10^4]$
20	$54.8121419(72)$	$4904.2443(16)$
	$[54.7(4)]$	$[4905(89)]$
30	$15.88750157(25)$	$667.244592(17)$

q	$F_d^{(5)}$	$F_d^{(6)}$
5	$4.90(39) \times 10^{22}$	$4.9(15) \times 10^{29}$
6	$1.092(30) \times 10^{16}$	$1.68(38) \times 10^{21}$
7	$1.363(14) \times 10^{13}$	$3.44(52) \times 10^{17}$
8	$2.625(11) \times 10^{11}$	$2.30(20) \times 10^{15}$
9	$1.8024(36) \times 10^{10}$	$7.67(37) \times 10^{13}$
10	$2.5155(25) \times 10^9$	$6.29(16) \times 10^{12}$
	$[2.40(26) \times 10^9]$	$[5.8(18) \times 10^{12}]$
15	$1.168612(78) \times 10^7$	$6.779(13) \times 10^9$
	$[1.170(59) \times 10^7]$	$[7.2(11) \times 10^9]$
20	$870078.5(88)$	$2.47889(69) \times 10^8$
	$[8.42(32) \times 10^5]$	$[2.33(16) \times 10^8]$
30	$55619.490(41)$	$7.44878(13) \times 10^6$

Table 6: Absolute value of the estimates of the energy cumulants $F_o^{(n)}$ for the ordered phase ($n = 3$–6). The values in the brackets are the data of the Monte Carlo simulations.

q	$F_o^{(3)}$	$F_o^{(4)}$
5	$2.1577(84) \times 10^9$	$7.368(33) \times 10^{15}$
6	$2.0467(28) \times 10^6$	$1.0698(22) \times 10^{11}$
7	$9.8469(57) \times 10^4$	$8.2777(91) \times 10^8$
8	$16460.8(46)$	$4.6939(32) \times 10^7$
9	$4905.23(73)$	$6.7098(35) \times 10^6$
10	$2018.31(17)$	$1.6071(11) \times 10^6$
	$[2031(26)]$	$[1.55(22) \times 10^6]$
15	$181.4445(19)$	$32878.80(86)$
	$[180.67(76)]$	$[2.93(20) \times 10^4]$
20	$57.05595(23)$	$5054.1460(86)$
	$[57.09(29)]$	$[4.79(22) \times 10^3]$
30	$16.7446548(22)$	$702.788233(56)$

q	$F_o^{(5)}$	$F_o^{(6)}$
5	$5.07(21) \times 10^{22}$	$5.15(46) \times 10^{29}$
6	$1.105(13) \times 10^{16}$	$1.775(60) \times 10^{21}$
7	$1.3691(65) \times 10^{13}$	$3.586(52) \times 10^{17}$
8	$2.6335(57) \times 10^{11}$	$2.356(16) \times 10^{15}$
9	$1.8084(19) \times 10^{10}$	$7.799(27) \times 10^{13}$
10	$2.5268(14) \times 10^9$	$6.367(12) \times 10^{12}$
	$[1.98(51) \times 10^9]$	$[2.8(14) \times 10^{12}]$
15	$1.185486(57) \times 10^7$	$6.8744(12) \times 10^9$
	$[0.92(15) \times 10^7]$	$[4.5(13) \times 10^9]$
20	$892352.53(68)$	$2.538205(72) \times 10^8$
	$[7.37(70) \times 10^5]$	$[1.38(26) \times 10^8]$
30	$58121.979(30)$	$7.760343(17) \times 10^6$